OXSAS software option for Thermo Scientific OES and XRF spectrometers   PRODUCT SPECIFICATIONS

ARLcom: package of result transmission solutions

ARLcom is a versatile optional package of Thermo Scientific OXSAS software to transmit manually or automatically analysis results using a variety of procedures, protocols and formats to best meet your needs. It can transmit analysis results online to up to 16 destinations via LAN network links or legacy RS-232 serial lines.

Data communication option

OXSAS can be fitted with ARLcom, a powerful and dependable transmission option that can transmit analysis results via network to applications running on other computers such as process computers, to database servers, to LIMS, etc. It can also send them to office computers enabling to treat them with word processor, spreadsheet or database applications such as the Microsoft® Office or OpenOffice® program suite. Legacy transmission mechanisms over serial lines is available too, whether you need to communicate to computers, to serial printers or to serial ASCII terminals

Flexible and secure communication solutions

- LAN Network TCP/IP: transmission solutions to computer applications via LAN Local Area Network using the TCP/IP protocol
- File Storage: transmission solutions to files located on local or network disks
- IP Printer: transmission of results to printers directly connected to a LAN network
- Compac: transmission solutions over RS 232 serial lines to computers using the Thermo Scientific Compac protocol
- Video/Printer: transmission solutions over RS 232 serial lines to printers or visual display terminals using formatted telegrams
- Alternate Destination facility automatically re-routes results to an alternative link if the main one can not be reached.

The high flexibility built in ARLcom suits the operation in real communication environment conditions. For instance, bufferisation or alternate destination is activated when the link is not available or has problems, when the receiving application is not listening, etc.
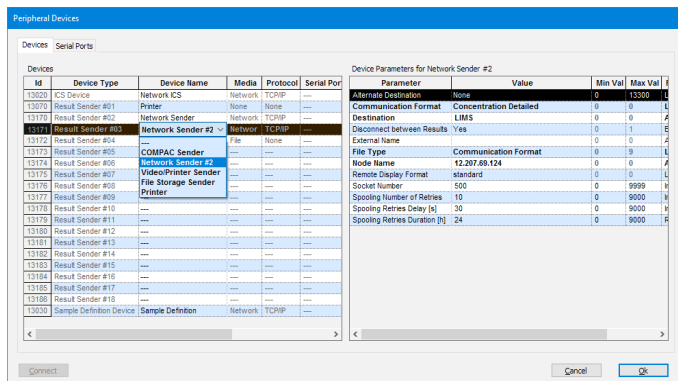
Defining links for result transmission is that powerful

Flexible transmission

Varied result transmission procedures

Results can be transmitted fully automatically after analysis completion. Alternatively, the user can control every transmission: the software proposes a list of destinations that can be amended online if necessary.

The lists of destinations can be set up for each category of your samples. You can also build automatic choices for the transmission destinations based on user definable criteria and using analysis information such as : sample identification, analysis parameter names, determined concentrations, flags, result status.

Results can also be transmitted upon request, for instance, results that are not regularly transmitted.

Stored results can also be transmitted; this allows among others the manual retransmission of results.

Generally, just the average concentration result would be transmitted, but individual measurements can also be sent. Besides the analyses of unknown samples, the measurements of control, setting-up, type standard and calibration samples can also be transmitted.

Transmission details, like the element list, order, precision, unit, etc. can be selected per analytical method, or can be defined for all methods in the transmission format.

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Result structures

OXSAS includes three types of transmission formats:

- Communication Formats, designed for transferring result data to online computer applications or databases
- Remote Display Formats. Thanks to their text formatting capability, they allow the display of results for direct human reading such as on passive terminals, on printers, etc,
- Report formats, that allow a coloured result print-out with customizable logo

A built-in tool enables to modifiy or create your own formats.

Secure transmission

Message Transmission Spooling

In case of unsuccessful transmission, the software temporarily stores the result message and automatically retries the transmission periodically. The retries delay and duration can be adapted for each destination.

The transmission spooling screen displays the results that failed to be transmitted with the name of their destination. The user can cancel the transmission retries per result, destination or for all results.

Alternate Destination

This function allows results to be sent to alternative destinations in case of transmission failure. The Alternate Destination facility is ideal for result transmission to computers having backup hardware for non-stop operation. If the main computer breaks down, the transmission fails and the system automatically re-routes the transmission to the backup system through Alternate Destination. The main destination is always used first, so the transmission is back to normal as soon as the main computer is running again.

Technical Notes

Alternate Destination can only be used for online communication mechanisms such as the LAN network TCP/IP, IP Printers or serial Compac destinations, as these communication mechanisms allow to detect the transmission failures. When used for File Storage destinations, it detects only when the destination folder is unreachable (e.g. if it does not exist, or if the drive is disconnected).

As alternative destination, you can select any of the destinations defined in your system provided they are of type: LAN network TCP/IP, File Storage, IP Printers or serial Compac.

LAN Network TCP/IP

The TCP/IP mechanism of ARLcom allows analysis results to be sent to computers using a LAN network access. The transmission is made in real time, task-to-task, from the analysis software to another application.

The TCP/IP solution offers a secure transmission: it allows immediate notification in the remote computer when a transmitted result is received. It also advises the operator if the result fails to be transmitted. In this event the result is spooled (stored temporarily), until the communication is restored. The result will then be re-transmitted automatically.

TCP/IP is a non-proprietary communication protocol used within most of today's networking applications, such as the Internet. The TCP/IP protocol is included in Windows® operating systems. It manages all the communication details. Just the node address of the receiving computer and a socket number for the communication have to be defined. A simple software program will be required on the destination computer to receive the message and extract the analytical result

Socket connection implementation

A schematic of the required program stages is shown in the diagram below.

Technical notes

- The destination computer requires the TCP/IP protocol installed and running
- The result reception program on the destination computer is not supplied
- Network hardware is not provided
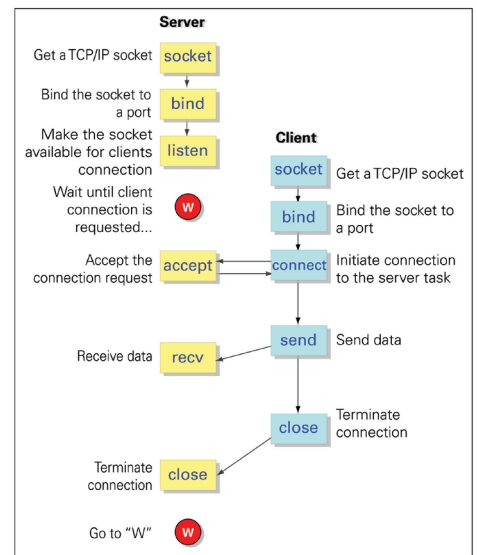
File storage on LAN Network or local disks

The File Storage mechanism of ARLcom allows writing analysis results to files either on the local disk or to network connected drives.

File Storage is an ideal mechanism of transmission to computers where an immediate response to process the result received is not required. The transfer is simple as the other application reads the result from a file without the need of a reception program. File Storage is also the perfect solution to send analysis results to a spreadsheet or to a database application like Microsoft® Excel, Access or OpenOffice®.

Flexible file definition

The name and path of the file can be specified per destination. You can set up OXSAS to either append results to previously sent ones in an existing file, or to overwrite the existing file, or to create a new file for each transmission. In this case, the file name has an incrementing numeric part, with a configurable number of digits.

Technical notes

- The networks supported are any network able to emulate a valid DOS path or an active directory for accessing a network drive, or a shared folder. Typical example are the Microsoft Networks available with Windows® Operating System
- Modification access right must be granted to the folder containing the destination file
- NFT (Network File Transfer), FTP (File Transfer Protocol) and NFS (Network File System) are not supported.

IP Printers

This is the solution to achieve a direct transmission of results to a printer directly connected to a LAN network. Such printers are fitted with a direct network connection and includes their own Print Queue system. To set up their connection in OXSAS, they simply need an IP address and a socket number. They shall accept direct formatted ASCII messages, since this printing mechanism does not use the Windows ® driver.

One of the key advantage of IP printers is that they are platform independent, i.e. they can be implemented in non-Microsoft networks and allow the remote printing of results, even automatically. It can be used as the modern solution in replacement to the Remote printers over legacy serial lines.

Serial Compac

Compac is the solution to send analytical results to computers via RS-232 serial lines.

It uses the Thermo Scientific Compac communication protocol described hereinafter. The messages are transmitted in ASCII and simple tasks are required on the receiving computer to support the protocol and extract the analytical result.

Compac offers a secure transmission: it allows immediate notification in the remote computer when a transmitted result is received. It also advises the operator if the result fails to be transmitted. In this event the result is spooled (stored temporarily), until the communication is restored. The result will then be re-transmitted automatically.

Compac protocol

This protocol is used to establish communication with a host computer and to detect any errors, as described below.
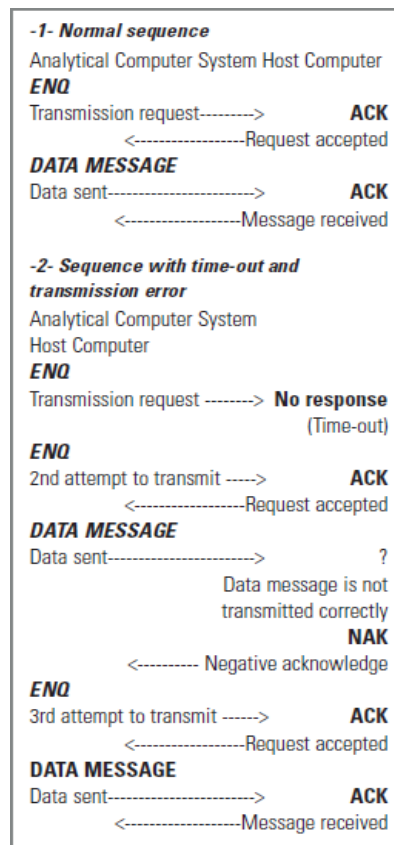
Frame structure

The structure of the data message is as follows (the characters marked with an "*" can be user defined):

- **STX** is always the first character of a data message and **ETX** is the last character
- **BCT (Byte count, 4 bytes)**: Total of bytes between the range as shown above: including the start of text control character, 4 bytes used for byte count calculation and the bytes composing message. To emulate old compac protocols, it is possible to configure the BCT to use only 3 bytes
- **DATA**: The data message containing the analytical result
- **CKS (Checksum, 3 bytes)**: Sum (modulo 256) of the values of each byte between the range as shown above: including the start of text control character, 4 bytes used for byte count calculation, and the bytes composing the message

- The **checksum** and **byte count** calculations exclude the checksum characters and **ETX Block Check Character (BCC) or Longitudinal Parity Character (LPC)**: This item is optional and is the sum of the respective rank bits of all characters of the message including the start of text and the end of text control characters and calculated as even parity (XOR function)

The following table lists the ASCII codes and the meaning of the different control characters used in the Compac protocol. Note that these are the default characters and they can be changed.

Name	Character	Dec.	Hex
ENQ	CTRL/E	5	05
ACK	CTRL/F	6	06
NAK	CTRL/U	21	15
STX	CTRL/B	2	02
ETX	CTRL/C	3	03

Serial Video/Printers

This solution is for the transmission of results to ASCII printers or ASCII visual display terminals. This simple mechanism allows the remote printing or display of results to legacy terminals connected to the OXSAS computer using RS-232 serial lines.

Utilities
Monitoring of the peripheral links and of the transmission performance

Monitoring the connections of OXSAS with the peripheral devices such as the destination computers and the printers makes their set up and troubleshooting very easy. Each peripheral link has its own screen where all exchanged messages are shown.

These monitoring windows allow to check the transmission of results: they show the successful, failed transmissions and errors with additional description if available.

Furthermore, the transmission events can be logged in log files and displayed in event monitoring windows. Distinct colors show the successful transmissions, the failures, the repetitions and low level information from the protocol layers. This greatly speeds up testing and fine tuning the communications.

ARLcom general technical notes

- Overall number of result destinations: maximum 16
- Cables, connectors and adaptation units supply and installation are not included.
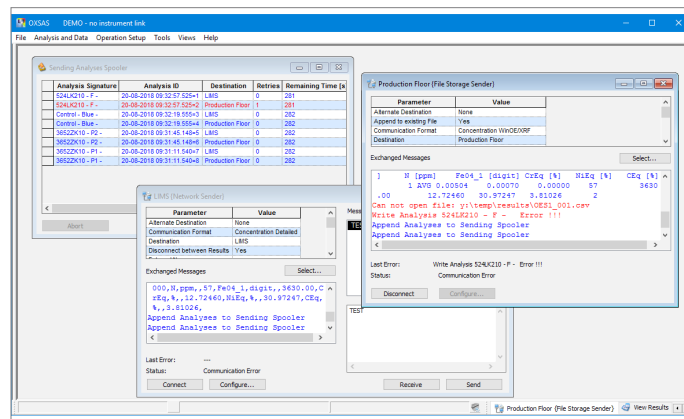
Easy setup and debugging thanks to powerful monitoring windows (one per device) and result spooler control screen

ARLcom technical notes for network links

The customer is responsible for the supply and installation of the protocol layer for the Thermo Scientific instrument computer (just like for any other PC of his network). However, the protocol layer is usually part of Windows® software, or of any other compatible software.

ARLcom technical notes for serial links

The total number of supported result destinations that uses a RS-232 serial link is limited to eight (this relates to the Compac and the Video/Printer transmission solutions). The result reception task on the host computer is not supplied by Thermo Fisher Scientific.

When necessary, extra communication lines are provided by mounting a MUX interface (2, 4 or 8 serial lines) in the computer.

The serial ports can have the following parameters:
- 7 or 8 data bits with 1 or 2 stop bits
- Parity odd, even or none
- Baud rate from 1200 to 115200 Baud
- Flow control: XON/XOFF, Hardware or none

Results structures

OXSAS includes two types of transmission formats:
- Communication Formats are designed for transferring result data to computers or to files
- Remote Display Formats: their text formatting capabilities allow displaying results in a format compatible for direct human reading such as on passive terminals, on printers, etc,

OXSAS is supplied with several default formats of each type, described hereinafter. However a built-in tool enables to create your own formats.

Computer communication format

These formats feature a layout with ASCII data separated by a delimiter. They are ideal for communication to computer applications running online and to databases. They are also convenient for transmitting results to other applications such

as spreadsheets or database programs (e.g. Microsoft® Excel, Access or OpenOffice®). The different formats differ from each other mainly through their content.

Concentration Detailed

This standard format features a very comprehensive content, mainly:

• Analysis Type

• Analysis Task, Method, Type Sandard, Grade

• 5 Sample identification Fields. More can be added if desired

• Element name, concentration, flag and unit

• Run information (run number, run in average, etc.) allowing the remote destinations to distinct the run measurement data when transmitted individually.

The date and time of the analysis are coded accorded to ISO8601 standard.

Refer to the table below for a full description of this format.

Concentration Short

This standard format contains only the most relevant data:

• Short sample identification (signature)

• Element name and concentration

The date and time of the analysis are coded according to ISO8601 standard.

Concentration WinOE/XRF

It provides the necessary compatibility with the previous WinOE and WinXRF. It is well comprehensive and includes all the run information necessary for the transmission of individual measurements. For more details on this format, see WinOE or WinXRF configuration manual.

Description of the standard OXSAS Computer Communication Formats

A ☑ in the table below indicates that this field is included in the corresponding standard format

Field No	Field Name	Format	Concentration Detailed	Concentration Short	Description, examples, etc.
F1.	Analysis type [4] (description)	Alphanumeric	✓		In the Concentration Detailed format, the analysis type is sent in full text (description), e.g. "Normal Analysis Unknown %". See the list of possible analysis type description hereafter[4]
F2.	Date and Time	YYYY-MM-DDTh:mm:ss	✓	✓	Date and time of analysis codes as per ISO8601 standard (with leading zero when necessary)
F3.	Task	Alphanumeric	✓		
F4.	Analytical Method	Alphanumeric	✓		
F5.	Type Standard	Alphanumeric	✓		Empty if it is not defined in the analysis result
F7.	Grade	Alphanumeric	✓		Empty if it is not defined in the analysis result
F7.	Runs Done	Numeric	✓		Total number of runs done during the analysis
F8.	Runs in Average	Numeric	✓		Real number of runs that were used to calculate the average
F9.	Run Number	Numeric	✓		Is 0 (zero) for the case the average is transmitted
F10.	Run Type[5]	Alphanumeric	✓		Type of the run contained in the message (description text)
F11.	Signature	Alphanumeric		✓	Short Sample identity. By default it is the concentration of the first three sample identity fields separated by a hyphen
F12.1	SID Value1	Alphanumeric	✓		Sample identity field 1
F12.2	SID Value2	Alphanumeric	✓		Sample identity field 2
F12.3	SID Value3	Alphanumeric	✓		Sample identity field 3
F12.4	SID Value4	Alphanumeric	✓		Sample identity field 4
F12.5	SID Value5	Alphanumeric	✓		Sample identity field 5
F13.	Number of elements	Numeric	✓	✓	Element Name (F14), Unit (F15), Flags (F16) and Value (F17) are repeated by the number of times given by the number of elements (F13). For the Short format, only the Element Name and Value are repeated
F14.	Element name	Alphanumeric	✓	✓	The element list and their order of transmission is the one defined in the Task (global validity) or in the analytical Method if a list per method is preferred (configurable by setup)
F15.	Element Unit	Alphanumeric	✓		The element unit is the one defined in the element format used in the Task or in the Method according to whether the first or the second is used (configurable by setup)
F16.	Element Flags[6]	Alphanumeric	✓		The possible flags are listed hereafter. An element can be marked by several flags simultaneously, in that case all set flags are sent
F17.	Element Value	Alphanumeric	✓	✓	The element precision is defined per setup. Possible precision formats are: fix number of decimals, fix number of significant digits, proportional number of decimals according to the actual concentration. Negative values are preceded by a minus sign.

Additional explanation notes on the standard OXSAS Computer Communication Formats

1. The ASCII comma "," character is used as a separator between the items in the message text. This character is replaced by an ASCII underscore "_" wherever it appears in the text

2. Unless specified in the format table above, fields are not truncated and are of variable length. They are transmitted as stored in the database. Note that the fields are limited to 255 characters in the database. Unused fields or fields whose content is empty are sent as an empty character followed by the field delimiter (by default it is the comma). They appear thus as two successive commas

3. Numerical fields have no leading nor trailing characters

4. The Analysis type describes the type of result being transmitted. Possible types are (code and its description):
   NA Normal Analysis Unknown %
   NI Unknown Intensity
   SI Standardization Initialize
   SU Standardization Update
   NX Normal Analysis with XRD phase
   AX Automation Production with XRD phase
   TI Type Standard Initialize
   TU Type Standard Update
   CA Calibration Standard
   CT Control Sample
   AP Automation Production Sample
   AD Automation Standardization Update
   AT Automation Type Standard Update
   AC Automation Control Sample
   QA Quantas Analysis Unknown %
   AV Metaverage (average of result averages)

5. "Run type" indicates the type of analytical run/result that the message contains:
   " " (empty field) Indicates an average value for an analysis not declared as "Bad sample". Only if run number=0
   B Indicates an analysis declared as "Bad sample". Only if run=0
   " " (empty field). This run is included in average. Only if the run is not an average
   x This run is not included in average. Only if the run is not an average.
   ? This run is a bad run. Only if the run is not an average
   B This run is a bad analysis.Only if run number=0 (Only for automation/SMS)
   A indicate an aborted analysis. Only if run number=0

6. Element flags field may contain one or more of the following characters:
   Flags qualifying individual runs only:
   *   Element not reproducible when reproducibility checking is being used
   }   Above the Pseudo-element validity range
   {   Below the Pseudo-element validity range
   ^   Channel overflow

v   Channel underflow
@   Spark-DAT overflow
~   Spark-DAT calculation error
_   Calculation unsuccessful (no final value)
n   Not selected in line choice selection

Flags qualifying individual runs and the average:
!   Below the Limit of Detection (LOD or DL)
)   Above the Calibration Range or the Validity Range of the Internal Standard
(Below the Calibration Range or the Validity Range of the Internal Standard
?   Pseudo-element calculation error
o   Has no Value

Flags qualifying the average only:
>   Above the grade top limit - positive values only. Also used when the result is above the outer top limit in the case the result is checked against two sets of limits (inner and outer)
<   Below the grade bottom limit - positive values only. Also used when the result is below the outer bottom limit in the case the result is checked against two sets of limits (inner and outer)
/   Above the grade inner high limit - positive values only. Used in case the result is checked against two sets of limits (inner and outer)
\   Below the grade inner limit - positive values only. Used in case the result is checked against two sets of limits (inner and outer). specification - positive values only
]   Above the upper Control or Specified Limit (UCL or USL)
[Below the lower Control or Specified Limit (UCL or USL)
D   Excessive drift (standardization mode)
Failed SPC test.
SPC:xxxx = SPC test result with code. (as per table below)

The xxxx number is the summation of the following test values (numbers given in hexadecimal):

1	Ignored (no tests applied)
2	Run of N above the mean
4	Run of N below the mean
8	Run of N increasing
10	Run of N decreasing
20	More than 90% in the middle 1/3
40	Less than 40% in the middle 1/3
80	Point outside UCL
100	Point outside LCL
200	Point outside USL
400	Point outside LSL
800	N (14) points alternating
1000	N (2) out of M (3) points outside 2 sigma
2000	N (4) out of M (5) points outside 1 sigma
4000	More than N (8) points outside 1 sigma
8000	Less than N (15) points within 1 sigma
10000	Homogeneity test

Example using the Concentration Detailed Format

```
Normal Analysis Unknown %, 2008-09-26T16:33:47,My
Task,My Method,,,1,1,1,,12345, Caster A,1,Stainless
Steel,99MP99999, 12,Si,%,,1.0636,S,%,,0.0208,P,%,
!<,0.0001,Mn,%, ,0.1193,Cr,%,<,15.9346,Mo,%,,0.930
5,V,%,, 0.0716,Cu,ppm,(,1.4,Ti,%,,0.0100,Sn,%,,0.17
07,Ni,%,,0.2546,C,%,,0.9912,
```

Same example using Concentration Short Format

```
2008-09-26T16:33:47,12345-Caster A 1,Si,1.0636,S,
0.0208,P, 0.0001 ,Mn,0.1193,Cr, 15.9346,Mo,0.9305,V,
0.0716,Cu,Ti,0.0100,Sn ,0.1707,Ni,0.2546,C,0.9912,
```

Advanced formatting capabilities of the Computer Communication formats

The standard OXSAS Concentration Detailed format is already well comprehensive. However, if your receiving computers request more capabilities, OXSAS can transmit other information, or you can format the result message differently in a very flexible way.

Additional Available Fields

In addition to the information that the Concentration Detailed format can already transmit, below is a list of the main other valuable fields that OXSAS can transmit:

- Additional Sample Identity Fields, if your sample ID structure includes more than 5 fields
- Sample Signature
- Batch name: name if the transmitted analysis was performed using a batch
- Grade limits per element against which the result was compared. If two grade limits set are used, both inner and outer limits can be sent
- Element channel name
- Element Standard Deviation (SD), Relative Standard Deviation (RSD) and Uncertainty , sent similarly to the individual runs
- Element Raw intensity, Element Corrected Intensity
- Modification reason, in case the result was modified by the user
- Transmission sequence number

Additional formatting flexibility

You can modify the standard OXSAS computer communication format. You can also create additional formats. This capability is useful if each of your destination computers or files request a distinct format. OXSAS provides for the following main formatting capabilities:

- As described above, you can extend your message with additional fields. But you can also remove practically any field in the standard telegrams to tailor your message as close as possible to your needs
- You can freely arrange the order of the fields with the exception to the elements fields (name, unit, flags, value) that must be placed at the end of the result messages
- Date and time format is configurable
- The element list, their order of transmission and their precision is the one defined in the Task (global validity) used for the analysis or in the Analytical Method if an element list per method is preferred. You can also define your own transmission format for the elements, i.e. the elements to transmit, their order and their precision
- OXSAS provides also for proportional precision formats: the number of decimals is a function of the actual result concentration, This function is configurable as well, i.e. the number and the limits of the concentration ranges and for each range the number of decimal and the unit. As a result of the above described capability, you can define a transmission format that uses a proportional element precision, however different from the display format
- Usually the element name, unit, flags and value are sent grouped per element and repeated for each element. You can also define to sent all element names grouped, then the unit of all elements, then the flags and finally the value of all elements
- Fields length can also be fixed. Although this solution is less and less used because of its inherent rigid structure, OXSAS can emulate such format that are still required by some process computers. If this option is selected, the field content is truncated if it is longer than the field length defined in the format. If the content is shorter, it is filled with trailing space to match the defined field length
- You can use another fields delimiter than the comma. e.g. a semi-colon, a space or a carriage return (cr)
- If your receiving computer requires it, you can define fields with a fix text content (e.g. for emulating a telegram header)
- You can also define an automatic format choice function. While in most case, the format is fix per destination, you can also select a different format depending on an information contained in the analysis.

This ultimate function is an example of the very sophisticated formatting flexibility of the OXSAS transmission functions that enables to cope with very complex requirements.

Remote display formats

They are formatted texts designed for easy display of results on printers or visual display terminals. Several layouts are available by default. They can also be used as templates allowing you to create your own formats.

- *Standard:* with detailed sample and analysis information for displaying concentration results individually, with or without Standard Deviation and Relative Standard Deviation
- *Grouped*: for displaying results grouped (aligned one under the other). Therefore, only a summary of the sample and analysis information are displayed to allow more space for the elements. This format fits particularly a charge progress investigation
- *Intensities:* to display intensities of analysis with SD and RSD
- *Setting-Up Samples:* this format includes the current value of the Setting-Up sample analysis, their last and their nominal values.

Advanced formatting capabilities

Like for the computer communication format, OXSAS provides for additional formatting functions for the remote display formats. In summary, they are:

- Possibility to modify existing formats, copy them or create new ones
- Ability to add or remove fields and to reorganize their order
- Date and time format is configurable
- The element list, their order of display and their precision is the one defined in the Task (global validity) or in the Analytical Method. You can also define your own element format. Proportional formats are supported too
- The element name, unit, flags and value are displayed grouped per element and repeated for each element. You can also define to display all element names grouped, then the unit of all elements, then the flags and finally the value of all elements
- Field length is configurable for a better reading (alignment of fields)
- You can define an automatic format choice.
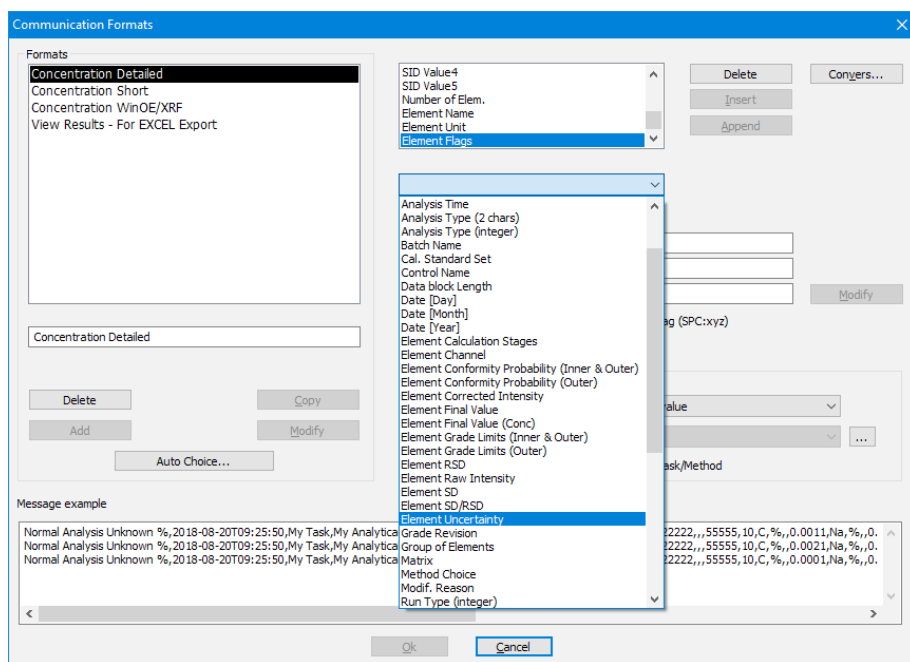
Very comprehensive tool to edit existing formats, copy them or create your own formats.

Find out more at **thermofisher.com/oxsas**

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